Semantic Breakthrough in Drug Discovery

Synthesis Lectures on the Semantic Web: Theory and Technology

Synthesis Lectures on the Semantic Web: Theory and Application is edited by Ying Ding of Indiana University and Paul Groth of VU University Amsterdam. Whether you call it the Semantic Web, Linked Data, or Web 3.0, a new generation of Web technologies is offering major advances in the evolution of the World Wide Web. As the first generation of this technology transitions out of the laboratory, new research is exploring how the growing Web of Data will change our world. While topics such as ontology-building and logics remain vital, new areas such as the use of semantics in Web search, the linking and use of open data on the Web, and future applications that will be supported by these technologies are becoming important research areas in their own right. Whether they be scientists, engineers or practitioners, Web users increasingly need to understand not just the new technologies of the Semantic Web, but to understand the principles by which those technologies work, and the best practices for assembling systems that integrate the different languages, resources, and functionalities that will be important in keeping the Web the rapidly expanding, and constantly changing, information space that has changed our lives.
Topics to be included:

- Semantic Web Principles from linked-data to ontology design
- Key Semantic Web technologies and algorithms
- Semantic Search and language technologies
- The Emerging "Web of Data" and its use in industry, government and university applications
- Trust, Social networking and collaboration technologies for the Semantic Web
- The economics of Semantic Web application adoption and use
- Publishing and Science on the Semantic Web
- Semantic Web in health care and life sciences

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ABSTRACT

The current drug development paradigm—sometimes expressed as, "One disease, one target, one drug"—is under question, as relatively few drugs have reached the market in the last two decades. Meanwhile, the research focus of drug discovery is being placed on the study of drug action on biological systems as a whole, rather than on individual components of such systems. The vast amount of biological information about genes and proteins and their modulation by small molecules is pushing drug discovery to its next critical steps, involving the integration of chemical knowledge with these biological databases. Systematic integration of these heterogeneous datasets and the provision of algorithms to mine the integrated datasets would enable investigation of the complex mechanisms of drug action; however, traditional approaches face challenges in the representation and integration of multi-scale datasets, and in the discovery of underlying knowledge in the integrated datasets. The Semantic Web, envisioned to enable machines to understand and respond to complex human requests and to retrieve relevant, yet distributed, data, has the potential to trigger system-level chemical-biological innovations. Chem2Bio2RDF is presented as an example of utilizing Semantic Web technologies to enable intelligent analyses for drug discovery.

KEYWORDS

drug discovery, semantic data integration, semantic analytics, semantic graph mining, semantic prediction

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